A Catalyst Uncovered

To many, the phrase "synthetic organic chemistry" probably sounds a bit dull. But this scientific field — the making, or "synthesizing," of carbon-based (i.e. organic) chemical compounds — has produced many, many products that we use every day. Examples include medicines, fuel, pesticides, paper, and even fabric for clothing. These breakthroughs are the results of many specific, intricate studies into how molecular reactions work.

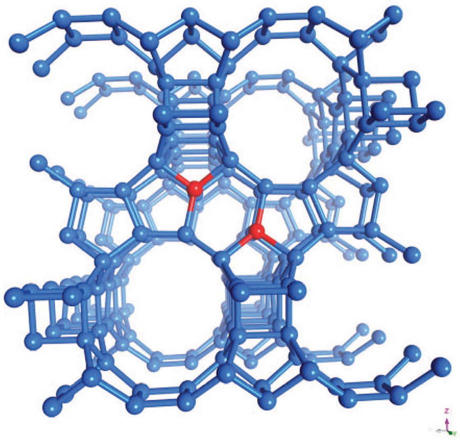
One such study was recently completed at the National Synchrotron Light Source. Led by chemist Simon Bare, a user scientist from the corporation UOP LLC, the group used x-rays to investigate a new, safe catalyst for an important type of reaction called Baeyer-Villiger (B-V) oxidation. Their results, reported in the September 21, 2005 edition of the *Journal of the American Chemical Society*, add a link to the long chain of discovery that leads, eventually, to better consumer and industrial products.

Authors (from left) Wharton Sinkler, Frank Modica, Laszlo Nemeth, Simon Bare, John Low. (Not pictured) Shelly Kelly, Susanna Valencia, and Avelino Corma

"Baeyer-Villiger oxidation is an important reaction in synthetic organic chemistry," said Bare. "Our aim is to make the reaction more stable and efficient by producing a better catalyst."

The B-V reaction involves transforming "ketones" – a class of organic solvents – into "esters," a type of compound formed by reacting an alcohol with an acid. Typically, this transformation is catalyzed by a group of acids called peracids, but these compounds are inherently unstable and require caution when used in large amounts. In contrast, the catalyst Bare's group is studying is a silicon-based mineral compound known as Sn-β-zeolite. In previous work, they showed Sn-β-zeolite to be an efficient, safe catalyst for B-V oxidation. Now, they have evidence that helps to explain, at the molecular level, *why* the catalyst is so successful.

Their results show that the effectiveness of Sn-β-zeolite as a catalyst depends on the "Sn" portion of the mineral — that is, the tin (Sn) atoms that are dispersed within the mineral's crystal structure. By shining x-rays at a Sn-β-zeolite crystal sample, they discovered that the tin atoms are not randomly placed within the crystal, but instead are found at regular, specific locations.



A representation of the Sn-β-zeolite structure as derived from the x-ray data Bare and his group collected. The red areas mark one possible Sn-atom pair.

"We believe that the uniform distribution of tin atoms produces sites in the mineral with uniform catalytic activity, which, in total, leads to the excellent overall behavior of the catalyst," said Bare. "However, we are still not sure why the Sn atoms are positioned so evenly in the crystal."

In future work, Bare's group will try to resolve this issue. In the meantime, they hope that this study illustrates that it is possible to synthesize catalysts with uniformly spaced reactivity sites. As long as those sites are easily accessible to the compounds taking part in the reaction, this approach has the potential to produce many effective, efficient catalysts.

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For more information, see: S.R. Bare, S.D. Kelly, W. Sinkler, J.J. Low, F.S. Modica, S. Valencia, A. Corma, and L.T. Nemeth, "Uniform Catalytic Site in Sn-β-Zeolite Determined Using X-ray Absorption Fine Structure," J. Am. Chem. Soc., ***127(37)****, 12924-12932 (2005).*

— Laura Mgrdichian